

trans-5-Ethylidene-bicyclo[2.2.1]hept-2-ene

Inchi: InChI=1S/C9H12/c1-2-8-5-7-3-4-9(8)6-7/h2-4,7,9H,5-6H2,1H3/b8-2+
InchiKey: OJOWICOBYCXEKR-KRXBUXKQSA-N
Formula: C9H12
SMILES: CC=C1CC2C=CC1C2
Mol. weight [g/mol]: 120.19
CAS: 28304-67-8

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-----------------|---------|----------------|
| chl | -5363.10 ± 1.80 | kJ/mol | NIST Webbook |
| gf | 209.72 | kJ/mol | Joback Method |
| hf | 150.40 ± 2.00 | kJ/mol | NIST Webbook |
| hfl | 106.50 ± 1.80 | kJ/mol | NIST Webbook |
| hfus | 14.78 | kJ/mol | Joback Method |
| hvap | 43.90 | kJ/mol | NIST Webbook |
| log10ws | -2.60 | | Crippen Method |
| logp | 2.529 | | Crippen Method |
| mcvol | 107.350 | ml/mol | McGowan Method |
| pc | 3333.53 | kPa | Joback Method |
| tb | 428.87 | K | Joback Method |
| tc | 638.10 | K | Joback Method |
| tf | 234.67 | K | Joback Method |
| vc | 0.414 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 295.25 | J/mol×K | 638.10 | Joback Method |
| cpg | 215.63 | J/mol×K | 428.87 | Joback Method |
| cpg | 231.35 | J/mol×K | 463.74 | Joback Method |
| cpg | 246.00 | J/mol×K | 498.61 | Joback Method |
| cpg | 259.64 | J/mol×K | 533.49 | Joback Method |
| cpg | 272.35 | J/mol×K | 568.36 | Joback Method |
| cpg | 284.20 | J/mol×K | 603.23 | Joback Method |

| | | | | |
|-------|-----------|--------|--------|---------------|
| dvisc | 0.0004759 | Paxs | 428.87 | Joback Method |
| dvisc | 0.0006149 | Paxs | 234.67 | Joback Method |
| dvisc | 0.0005742 | Paxs | 267.04 | Joback Method |
| dvisc | 0.0005441 | Paxs | 299.40 | Joback Method |
| dvisc | 0.0005211 | Paxs | 331.77 | Joback Method |
| dvisc | 0.0005029 | Paxs | 364.14 | Joback Method |
| dvisc | 0.0004881 | Paxs | 396.50 | Joback Method |
| hvapt | 41.20 | kJ/mol | 381.00 | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C28304678&Units=SI |

Legend

| | |
|-----------------|---|
| chl: | Standard liquid enthalpy of combustion |
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfl: | Liquid phase enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |
| hvapt: | Enthalpy of vaporization at a given temperature |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

Latest version available from:

<https://www.cheméo.com/cid/70-443-2/trans-5-Ethylidene-bicyclo-2-2-1-hept-2-ene.pdf>

Generated by Cheméo on 2024-05-02 08:51:48.991658108 +0000 UTC m=+16929157.912235442.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.